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Modelling Concentration Profiles of Chemical Warfare Agents to Assess the Usefulness of Airborne Chemical Detectors

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ABSTRACT

The concept of airborne chemical point-detectors followed from the increasing availability of unmanned aerial vehicles (UAVs). The atmospheric hazard modelling program HPAC (Hazard Prediction and Assessment Capability) is used to examine the vertical concentration profiles that a UAV borne detector will be exposed to in military scale releases of chemical warfare agents. The airborne chemical detection capability obtained from a point-detector with a detection limit of 0.1 mg/m^3 borne by a UAV operating at 50 metres above ground level is shown to have very limited application.

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Executive Summary

The increasing availability of Unmanned Aerial Vehicles (UAVs) for service with the Australian Defence Force (ADF) has prompted much discussion about the best uses for such technology. One possibility is to equip a UAV with a chemical detector to detect releases of chemical warfare agents.

To obtain a better understanding of the capability that the UAV-borne detector would offer, DSTO modelled a series of military-scale releases of chemical warfare agents (CWA) using the Hazard Prediction and Assessment Capability (HPAC). Both persistent and non-persistent agents were modelled under various atmospheric conditions, and their concentration profiles examined at a variety of points downwind at heights of 50 and 100 metres above the ground. This report assumes the detector will respond to a CWA concentration of $0.1 \ mg/m^3$ and that the UAV can operate at 50 metres above ground level.

Non-persistent and semi-persistent agents were detectable under most conditions for a period of around 30 to 45 minutes post-release. The more persistent agents that were modelled displayed different plume characteristics, but were either not detectable at 50 or 100 metres, detectable over a small area or detectable for a short time at any point. A deliberate release of a chemical agent for purposes of terror is likely to involve a much smaller quantity of agent and will not be detectable with UAV-borne detectors.

The UAV-borne chemical detector will not be able to map ground contamination. For the persistent agents sulphur mustard and the nerve agent VX, liquid deposited to the surface remains a hazard for 5 hours and 9 days respectively, however the UAV can detect these agents for only 35 minutes and 5 hours respectively.

The modelling undertaken suggests there is limited application of UAV-borne chemical warfare agent detectors unless they can operate more slowly and at a lower altitude than assumed in this report.

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Alexander Hill graduated from the Royal Melbourne Institute of Technology with a B. Sc. (Hons.) in mathematics in 2001. He has been employed at the Platform Sciences Laboratory since February 2002 in the CBR Hazard Modelling area.

Contents

1. Introduction

Being able to detect chemical warfare agents (CWA) quickly and to define the scale of contamination resulting from their use is vital during military operations. The use of networks of chemical agent detectors to increase the chance of detection has been considered, but usually only at ground level. A consequence of the introduction of Unmanned Aerial Vehicles (UAVs) is the possibility of aerial detection of chemical agents.

To determine the usefulness of air-borne detectors, DSTO undertook some dispersion modelling of various chemical agent releases for a range of atmospheric conditions. This modelling is intended to assist Australian Defence Force (ADF) understanding of the use of UAVs as air-borne chemical detectors.

2. The HPAC Model

The Hazard Prediction and Assessment Capability (HPAC) is an atmospheric dispersion model that has been developed by the Defense Threat Reduction Agency (DTRA) to model the releases of chemical, biological and radiological (CBR) material associated with the use of weapons of mass destruction (WMD). It is widely used in the United States and provided support to the Salt Lake City winter Olympic Games in 2002 and the US Presidential Inaugurations in 1997 and 2001.

In Australia, HPAC has been used to support the security of the Commonwealth Heads of Government Meeting (CHOGM) in 2002. Its users include DSTO and the Incident Response Regiment (IRR), as well as several state fire and emergency services.

HPAC uses a Gaussian puff dispersion model engine known as SCIPUFF (Second Order Closure Integrated PUFF model) to model the dispersion of clouds of liquids, vapours and particulates. The plume of chemical agent discussed in this report is modelled as small puffs of material with an associated probability distribution relating concentrations for various points in time and space. More information on the SCIPUFF model is contained in the SCIPUFF technical documentation [1].

3. Overview of Modelling Undertaken

HPAC was used to model vapour dispersion of military scale releases of four chemical warfare agents (CWA): Sarin (GB), Soman (GD), Sulphur Mustard (HD) and the persistent nerve agent VX. Of these agents, GB is the most volatile and hence not persistent, GD is slightly persistent and HD and VX are highly persistent. Consequently, liquid GB would evaporate very quickly, GD more slowly and HD and VX would evaporate very slowly. More details on the properties of chemical warfare agents are available from open literature publications [2].

Atmospheric conditions play a major role in the dispersion of the agent and so three distinct situations were used. These were based loosely on the Pasquill Gifford Turner

(PGT) atmospheric stability index. PGT stabilities A, D and F were used to simulate unstable, neutral and stable conditions respectively. Unstable conditions usually occur on a clear, fine day with low wind speed and result in fast dispersion of material. Neutral conditions were modelled as a cloudy day with high wind speeds. A clear night with low wind speeds usually result in relatively stable conditions and very slow dissipation of the vapour hazard. More details on the PGT index can be found in a review of agent dispersal prediction, published as a DSTO general document [3]. These conditions assume a constant wind speed and temperature, and a fairly smooth terrain; hence they are not particularly realistic and usually result in "worst-case" dispersion results. A full list of meteorological parameters chosen can be found in Appendix A.

The release is of approximately 1 tonne of liquid chemical dispersed using thirty-two 100 kg aerial bombs, each containing 34 kg of agent. The bombs are spread over a circular area with a diameter of 370 metres, giving an average deposition quantity of approximately 10 g/m² (a standard level in chemical defence work). Hypothetical detection devices are placed at ten distances downwind at 50 and 100 metres above ground level (AGL), and concentrations are measured every 30 seconds. See Appendix A for more details on the release assumptions.

For the purpose of this report, it is assumed that a detector will respond if exposed to a CWA concentration of greater than 0.1 mg/m^3 for more than 30 seconds.

4. Results and Discussion

The modelling results were analysed and are summarised in Table 1 below. Note that downwind and crosswind distances are approximate due to the limited number of detectors modelled.

Crosswind distances were included to give an indication of the area that contains detectable concentrations at the two heights above ground level. The maximum downwind distances mentioned in Table 1 do not necessarily represent the size of the cloud at any point in time, but the maximum distance downwind that detectable concentrations travel. This is illustrated further below.

Also included in Table 1 are estimates of the time for which there exists a liquid agent hazard from ground contamination. Ground contamination times are much larger than the detection times for the persistent agents due to the lower volatility of these agents. The assumption of constant conditions is not valid for more than a few hours in general, so to get a more accurate estimate of the time that VX remains a liquid contamination hazard, HPAC's built-in database of historical weather was used. Information on the historical weather database can be found in the HPAC User's Guide [4].

As expected, the more persistent agents are detectable for longer, but do not travel as far downwind or crosswind. As the atmosphere becomes more stable, less vertical mixing occurs, dispersion is slowed and this results in lower concentrations at 50 and 100 metres above the surface. It is clear that under stable conditions (which occur on a still

night and are characterized by a temperature inversion) it is unlikely that a concentration above the 0.1 mg/m³ detection limit will occur.

Table 1: Summary of modelling results

Atmospheric Stability & Agent	Height AGL (m)	Time Detectable (min)	Maximum Downwind Distance (km)	Maximum Crosswind Distance (km)	Max. Ground Contamination Time (min)
Unstable - GB	50	0 - 30	< 5	< 2	< 5
	100	0 - 30	< 5	< 2	
Unstable - GD	50	0 - 25	< 3	< 2	< 10
	100	1 - 25	< 3	< 2	
Unstable - HD	50	0 - 35	< 15	< 1	< 40
	100	1.5 - 30	0.5 - 15	< 1	
Unstable - VX	50	0 - 300	< 0.5	< 0.5	~ 9 days
	100	0 - 150	< 0.5	< 0.5	
Neutral - GB	50	0 - 50	< 30	< 2	< 5
	100	0 - 50	< 30	< 2	
Neutral - GD	50	0 - 45	0.1 - 30	< 2	< 10
	100	1.5 - 45	0.5 - 30	< 2	
Neutral - HD	50	0 - 35	< 15	< 1	< 40
	100	0 - 35	< 15	< 1	
Neutral - VX	50	Not detectable	N/A	N/A	~ 9 days
	100	Not detectable	N/A	N/A	
Stable - GB	50	13 - 95	< 20	< 3	< 10
	100	Not detectable	N/A	N/A	
Stable - GD	50	5 - 80	< 15	< 2	< 50
	100	Not detectable	N/A	N/A	
Stable - HD	50	Not detectable	N/A	N/A	< 300
	100	Not detectable	N/A	N/A	
Stable - VX	50	Not detectable	N/A	N/A	~ 9 days
	100	Not detectable	N/A	N/A	

4.1 Non-persistent and Semi-persistent Agents

Based on this dispersion modelling, the UAV-borne chemical detector would encounter detectable concentrations of non-persistent and semi-persistent agent for perhaps 30 minutes after the release. Under neutral conditions, where wind speeds are higher, the time may be up to around 45 minutes, although the time that detectable concentrations exist at any point is around 5 minutes.
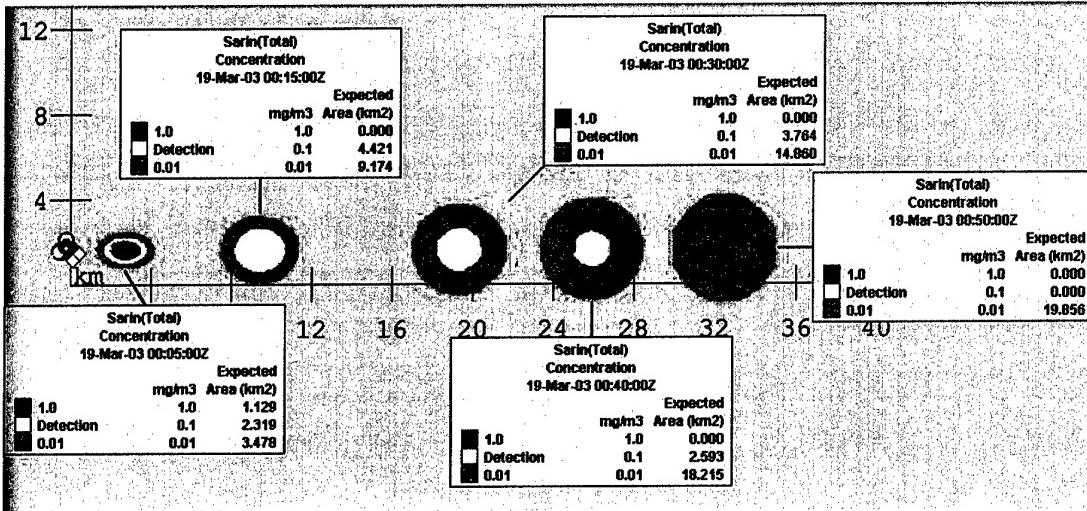
Figure 1: Contour plot of sarin release under neutral conditions at 50 metres AGL

Figure 1 shows a series of HPAC contours for the sarin release under neutral conditions (for 5, 15, 30, 40 and 50 minutes after release, reading from left to right). The cloud travels very quickly due to the high wind speed associated with neutral conditions, in this case 5 m/s. Note that the 'detection' contour never reaches more than 2.5 kilometres in diameter, and is roughly circular.

If we take the Aerosonde UAV as an example (the company website [5] contains specifications and other information on the Aerosonde UAV), we might expect the minimum speed of the UAV to be 18 m/s. Not taking into account the movement of the cloud (approximately 12 m/s at 50 metres AGL) and assuming a constant bearing, the Aerosonde UAV will have less than 2.5 minutes to detect the agent. Keeping in mind that detectable concentrations are present for less than 50 minutes, and the rapid downwind movement of the agent cloud, a UAV-borne detector will have only a limited opportunity to detect the agent. Similar trends occurred in the results of modelling GB and GD under all conditions. Figure 1 also demonstrates that the detection of the agent cloud provides little information on the location of the release, other than the relative direction, and no information on the level of ground contamination.

4.2 Persistent Agents

4.2.1 Sulphur Mustard

The concentration profiles of the two persistent agents modelled are quite different. Sulphur mustard concentrations are detectable for around 30 minutes and travel in a narrow plume up to 15 kilometres from the release point for neutral and unstable conditions. Under stable conditions, usually associated with a clear evening with little wind, mustard concentrations at 50 and 100 metres AGL never reach a detectable level. Figure 2 below shows an example HPAC contour plot of sulphur mustard concentrations.

Mustard(Total)
Concentration
19-Mar-03 00:20:00Z

	mg/m3	Expected Area (km2)
1.0	1.0	0.022
Detection	0.1	7.037
0.01	0.01	25.126
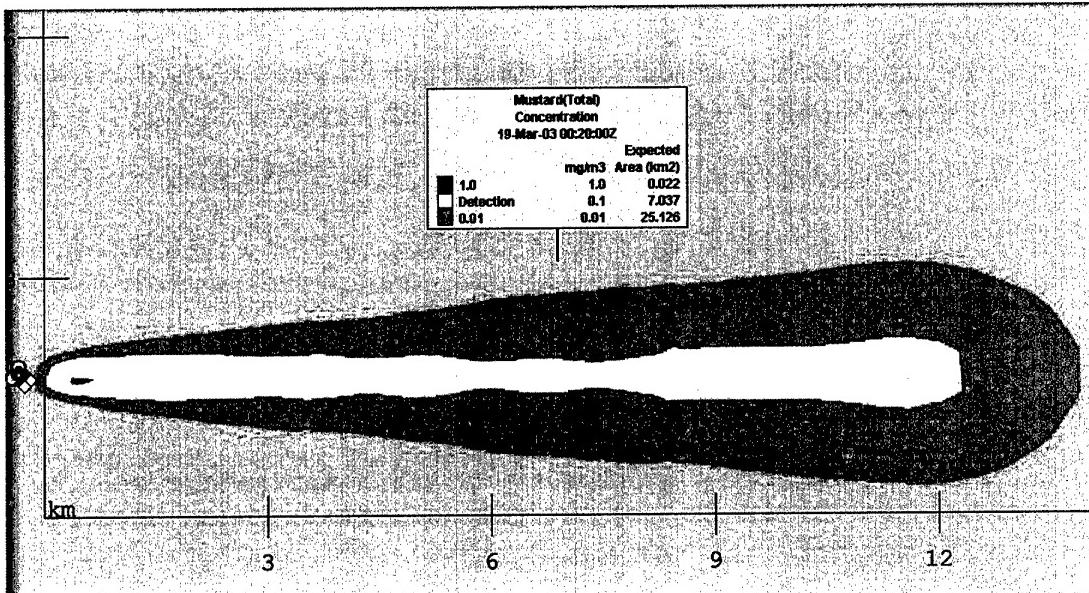
Figure 2: Contour plot of sulphur mustard release under unstable conditions at 50 metres AGL

Like the non-persistent and semi-persistent agents modelled (sarin and soman respectively), sulphur mustard contours are detectable for around 30 minutes after release for neutral and unstable conditions. Under stable conditions however, sulphur mustard is not detectable at any time after the release at 50 and 100 metres above the surface due to a combination of low volatility and limited vertical mixing in the atmosphere.

Figure 2 shows the concentration field at 20 minutes after the release in unstable conditions and demonstrates the very different structure of the concentration field when compared with that of sarin and soman. Note the long and thin shape of the detectable concentration contour, which extends 12 kilometres downwind, as opposed to the small transient cloud demonstrated in Figure 1. Using the Aerosonde UAV as an example again, we expect that travelling with the wind at 18 m/s, the detector may be exposed to a concentration greater than 0.1 mg/m3 for up to 10 minutes. The crosswind cloud width is less than a kilometre however, so the exposure time would be less than a minute if the UAV flies perpendicular to the wind. While the opportunity to detect the agent cloud is greater than for the less persistent agents GB and GD, detectable concentrations are present for only 30 minutes.

4.2.2 Persistent Nerve Agent VX

The nerve agent VX is only detectable during unstable conditions, such as might be experienced during a fine day with little wind. Under these conditions detectable concentrations exist for up to 5 hours, but only within 500 metres of the release. Maximum concentrations for VX under neutral and stable conditions vary from 0.06 mg/m^3 for neutral conditions and 50 metres AGL to less than 0.0001 mg/m^3 at 100 metres AGL under stable conditions.
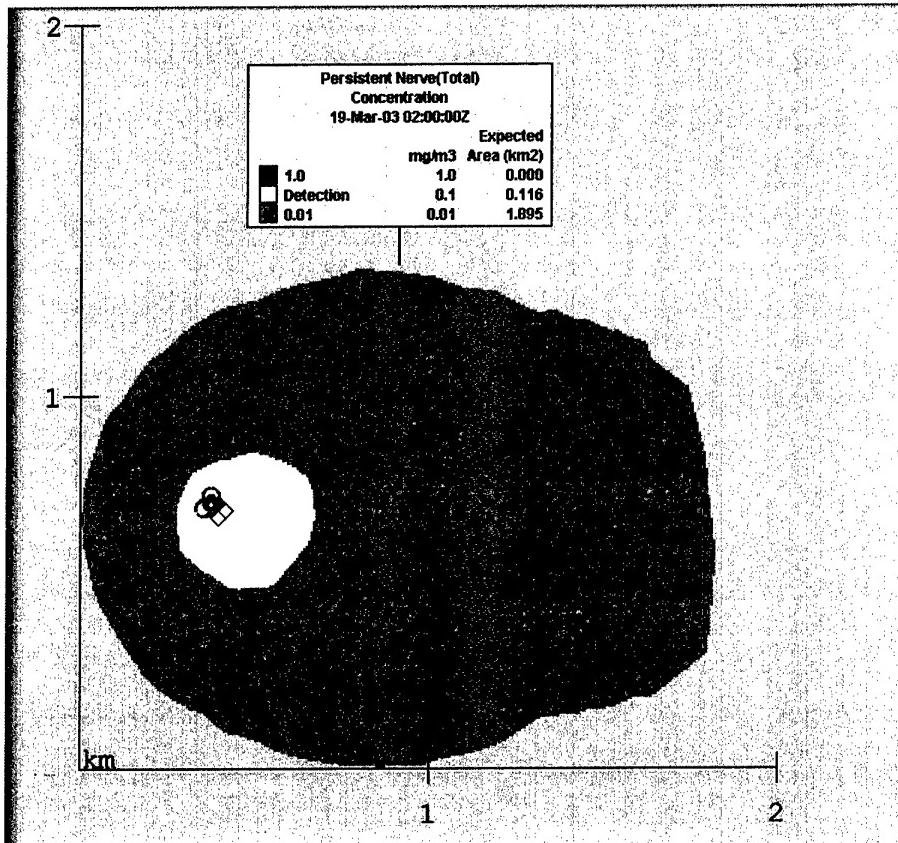
Figure 3: Contour plot of persistent nerve agent VX released under unstable conditions at 50 metres AGL

Figure 3 shows the VX concentration field at 50 metres AGL 2 hours after the release in unstable conditions. Note that in this case, detectable concentrations of VX persist for up to five hours. The structure of the contour differs from all previous agents examined, with the detectable cloud being approximately circular with a diameter of less than 500 metres, and not moving (in detectable quantities) downwind of the release.

Again using the Aerosonde UAV as an example of likely UAV speeds, we would expect an exposure time of less than thirty seconds. In this report we have assumed that the detector will alarm if exposed to a concentration of 0.1 mg/m3 for at least 30 seconds, so the UAV-borne detector may not detect the presence of VX even if flown directly across the cloud.

It is also worth noting that the ground contamination for this release scenario is likely to persist at hazardous levels for around 9 days. A UAV-borne chemical detector will not be able to map this hazardous ground contamination.

4.3 Comparing Concentration Over Time to Measure Persistency

Some comparison was also made of the concentration profile at a point over time for various agents. Figure 4 illustrates the effect of increasing the persistency of the agent modelled under neutral conditions.
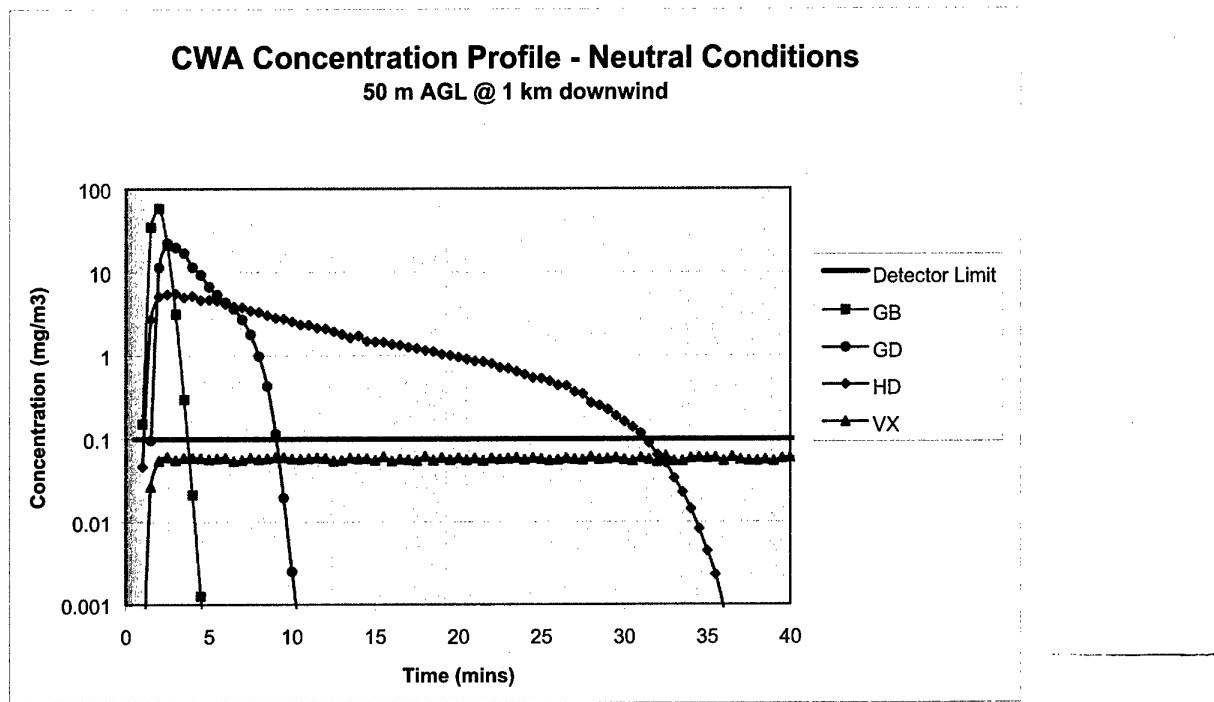
Figure 4: Concentration versus time plot for various chemical warfare agents at 50 metres above the surface and 1 kilometre downwind from release point under neutral atmospheric conditions.

Figure 4 clearly shows higher concentrations and fast dispersion for the less persistent agents such as GB and GD, and lower concentrations for a long period of time for the more persistent agents such as HD and VX.

5. Practical Considerations in Transient Cloud Mapping

The releases examined in this report are all very large, such as would be associated with the use of chemical warfare agents on the battlefield. To deliver the quantities of agent for a release of the scale modelled in this report would require large artillery, rockets or heavy aerial bombing, and these are likely to be easily recognised on the battlefield. Terrorist use of chemical agents is likely to involve much smaller quantities and it is unlikely that a detector on a UAV operating at 50 metres AGL would be able to detect these types of releases.

For those combinations of agents and atmospheric conditions investigated in this report that result in a concentration of greater than 0.1 mg/m3, the crosswind distances are usually no more than 2 kilometres. This means that the faster the UAV travels, the less likely the attached chemical detector is to remain in the chemical warfare agent cloud long enough to generate a response. Similarly, the higher above the surface that the UAV is flying, the lower the concentrations it will be exposed to. It is also important to note that after alarming, many current chemical detectors will need a period of time to 'clear down' before they are ready to detect again. High concentrations of material result in longer clear down times. In Figure 1 the volatile agents such as GB are at concentrations more than 100 times higher than the minimum for detection, and this may result in the temporary loss of detector capability.

6. Conclusion

This report has shown that a UAV-borne chemical detector would be able to detect transient plumes from large-scale releases of most chemical warfare agents, but only for the first 30 minutes after release and in a limited range of atmospheric conditions. Highly persistent agents, such as the nerve agent VX, may be detectable for longer under convective conditions (usually associated with daytime conditions with little wind), but is not detectable for neutral and stable conditions. There appears to be limited military application for this capability, since battlefield releases of CWA would be identified by other sources much more quickly and efficiently. Given the speed at which a UAV is likely to operate and the transient nature of the cloud of agent, a UAV-borne detector is likely to have limited use as a hazard-warning tool.

A chemical detector mounted on a UAV will not be able to map the contamination of the ground with liquid agent. Persistent agents will remain a liquid hazard on the surface for a long time, but will be detectable only briefly due to their low volatility. For example, sulphur mustard is likely to remain a hazard from liquid contamination of the ground for several hours but is detectable for less than 30 minutes. The nerve agent VX can be detected under some conditions for up to 5 hours, but the corresponding time at which ground contamination remains a hazard is estimated at 9 days.

The scenarios modelled tend to indicate that unless the UAV can operate below 50 metres and at lower speeds, a UAV-borne chemical warfare agent detector would have limited applications in the field. The use of an unmanned helicopter is not likely to become a solution, as the rotary action will tend to re-aerosolise any ground contamination, creating a secondary plume. A more sensitive detector would also improve the usefulness of this capability.

7. References

[1] Sykes, R I, Parker S F, Henn, D S, Cerasoli, C P, Santos, L P, PC-SCIPUFF Version 1.2PD Technical Documentation, ARAP Report No 718, Titan Corporation Research and Technology Division, Princeton, NJ, September 1998

[2] Ali, J, Rodrigues, L, Moodie, M, Jane's US Chemical-Biological Defense Guidebook, 1997, Janes Information Group, Alexandria, Virginia, p 49

[3] Gailis, R, Fulford, G, Agent Dispersal Prediction, DSTO-GD-0293, 2001, DSTO Aeronautical and Maritime Research Laboratory, Fishermans Bend, VIC p 16

[4] Hazard Prediction and Assessment Capability (HPAC) User's Guide Version 4.0.3, 9th May 2003, HPAC-UGUIDE-01-RBC1, Science Applications International Corporation, San Diego, CA, p 7.8.2

[5] The Aerosonde System, Aerosonde Pty Ltd, viewed 29th May 2003, <http://www.aerosonde.com/downloads/the_aerosonde_system.doc>

Appendix A: Parameter Selections and Justification

Release:
Munition Type	= 100 kg bombs	
Delivery System	= 4 Aircraft x 8 bombs	
Agent	= GB, GD, VX, HD	
Mass of Load	= 34 kg	(Military strike)
MMD[1]	= 500 μm	(HPAC default)
Sigma D[2]	= 2	(HPAC default)

Dissemination Efficiency	= 100 %	
Agent Purity	= 100 %	
Vapour Fraction	= 0 %	
Liquid Fraction	= 100 %	(All agent initially in liquid form)
Total Release Mass	= 34 kg	
HOB (AGL) [3]	= 15 m	(HPAC default, 2m for GB[4])
Initial Size	= 8 m	(Size of initial burst cloud, HPAC default)
Number of Bombs	= 32	
Spread (diameter)	= 370m	(Gives approx 10g/m2)

Location:
Latitude	= -37.0 N	
Longitude	= 145.0 E	
Date	= 19/03/03	
Time	= 0000 UTC	(1000 local)

Weather:
Wind Speed	= 1 m/s	(Assumed constant for 30 minutes)
Wind Direction	= 270°	(Assumed constant for 30 minutes)
Temperature	= 20°C	(Assumed Constant)
Surface Moisture	= Normal	(Affects Boundary Layer Approximations)
Surface Type	= Grassland	(Affects Boundary Layer Approximations)
Cloud Cover	= Clear (5 %)	(Affects Boundary Layer Approximations)
Precipitation	= None	(Rain would remove hazard)
Terrain	= Not included	(Assumed flat)
Landcover	= Not included	(Assumed grassland)

Boundary Layer Parameters:
Bowen Ratio	= 0.9	(Typical of summer/autumn & grassland)
Albedo	= 0.2	(Typical of summer/autumn & grassland)
Surface Roughness	= 0.1m	(Smooth surface)

PGT Stability Index:
Atmospheric Stability	= Unstable, A	(Land lapse, lots of vertical mixing)

Calculation Parameters:
Max Time-step	= 30 sec	
Output Interval	= 1 minute	(High resolution)

Length of Run   = Up to 12 hours
Sampler Locations   = 0, 0.1, 0.2, 0.5, 1, 2, 5, 10, 20 & 50 kilometres downwind

The above parameters are for Unstable conditions for each chemical warfare agent. For
neutral conditions, cloud cover was changed to 95%, wind speed to 5 m/s, and PGT
stability index to D. For stable conditions, release time changed to 1400 UTC (0000 local),
wind speed to 1 m/s, cloud cover to 5% and stability index to F.

Notes: 1) – MMD – Mass Mean Diameter, a measure of liquid droplet size

          2) – Sigma D – Measure of variability in MMD (standard deviation)

          3) – HOB – Height of Burst; AGL – Above Ground Level

          4) – HOB default is only 2m for GB, as it is highly volatile; HOB default is 15m for
          other three agents, as they are more persistent.

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19. ABSTRACT

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